Superfast front propagation in reactive systems with anomalous diffusion

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(February 8, 2008)

We study a reaction diffusion system where we consider a non-gaussian process instead of a standard diffusion. If the process increments follow a probability distribution with tails approaching to zero faster than a power law, the usual qualitative behaviours of the standard reaction diffusion system, i.e., exponential tails for the reacting field and a constant front speed, are recovered. On the contrary if the process has power law tails, also the reacting field shows power law tail and the front speed increases exponentially with time. The comparison with other reaction-transport systems which exhibit anomalous diffusion shows that, not only the presence of anomalous diffusion, but also the detailed mechanism, is relevant for the front propagation.

Pacs: 05.45.-a, 47.70.Fw

The propagation of fronts generated by a reaction-transport system has a considerable interest in a large number of chemical, biological and physical systems [1]. One important model is the advection-reaction-diffusion equation (ARD)

$$\partial_t\theta + (\mathbf{u}\cdot\nabla)\theta = D_0\nabla^2\theta + f(\theta)/\tau, \qquad (1)$$

where D_0 is the molecular diffusivity, $\mathbf{u}$ is a given incompressible velocity field and the term $f(\theta)/\tau$ describes the production process, whose typical time is τ. The scalar field θ represents the fractional concentration of the reaction's products: $\theta = 1$ indicates the inert material, $\theta = 0$ the fresh one and $0 < \theta < 1$ means that fresh materials coexist with products. Usually one considers $f(\theta)$ with an unstable fixed point at $\theta = 0$ and a stable one at $\theta = 1$ [2,3].

Eq. (1) was originally introduced (in the case $\mathbf{u} = \mathbf{0}$) by Fisher and Kolmogorov, Petrovskii and Piskunov (FKPP) with $f(\theta) = \theta(1-\theta)$ [4]. Then, the ARD equation has been widely studied in the context of combustion, population growth, aggregation and deposition.
In absence of stirring ($\mathbf{u} = \mathbf{0}$) it can be shown that a front, replacing the unstable state by the stable one, moves with a speed $v_0 = 2\sqrt{D_0 f'(0)/\tau}$. This result is valid whenever $f(\theta)$ is a positive convex function ($f''(\theta) < 0$) with two fixed points. For a non-convex production term only an upper and lower bound for v_0 can be provided [2].
A more interesting situation occurs in the presence of stirring ($\mathbf{u} \neq \mathbf{0}$): the front propagates with an average limiting speed v_f larger than v_0. Under general conditions [7,8], the advection-diffusion equation, i.e., $\partial_t\theta + (\mathbf{u}\cdot\nabla)\theta = D_0\nabla^2\theta$, has the same asymptotic feature of a diffusion equation. One has that the field $\langle\theta\rangle$ (obtained with an average on volumes of linear size much larger than the typical length of $\mathbf{u}$) at large time obeys a Fick equation:

$$\partial_t\langle\theta\rangle = \sum_{i,j} D^e_{ij}\partial^2_{ij}\langle\theta\rangle \ . \qquad (2)$$

The eddy diffusion coefficients, D^e_{ij}, contain all the (often non-trivial) effects of the velocity field $\mathbf{u}$. Eq.(2) states that a test particle described by the Langevin equation:

$$\mathrm{d}\mathbf{x}/\mathrm{d}t = \mathbf{u} + \sqrt{2D_0}\boldsymbol{\eta} \qquad (3)$$

where $\boldsymbol{\eta}$ is a white gaussian noise with $\langle\eta_i\rangle = 0$ and $\langle\eta_i(t)\eta_j(t')\rangle = \delta_{ij}\delta(t-t')$, follows, at large time, a Brownian motion $\langle(x(t)-x(0))^2\rangle \simeq 2D^e_{11}t$, where we suppose that the first coordinate is the propagation direction. As a consequence of the asymptotic diffusive behaviour it is possible to show that the front propagates with a finite $v_f \leq 2\sqrt{D^e_{11}f'(0)/\tau}$ [5,6].
If the conditions for the validity of standard diffusion do not hold, anomalous diffusion can be observed, i.e.,

$$\langle(x(t)-x(0))^2\rangle \sim t^{2\nu} \qquad (4)$$

with $\nu > 1/2$ (super-diffusion) [8,9]. There are at least three known mechanisms leading to the anomalous diffusion [7–13]:
a) an infinite variance of the velocity field $\mathbf{u}$;
b) an infinite memory, i.e., the velocity-velocity correlation function has a non integrable tail;
c) an effective diffusion coefficient increasing with the distance between two particles (in the case of relative diffusion).

Mechanism **a)** is perhaps the simplest one and Lévy flights belong to this class [10,11]. Some deterministic maps (e.g., the standard map for specific values of the control parameter) can produce super-diffusion according to mechanism **b)** [12]. An important example of mechanism **c)** is given by the fully developed turbulence [13]. There, the relative dispersion of two particles at distance R is described by a diffusion equation with an effective diffusion coefficient $D^e \sim R^{4/3}$.

It is natural to wonder about the effects of the super-diffusion for the front propagation. In this letter we discuss mechanism **a)**. The evolution equation of θ has the structure:

$$\partial_t \theta = \hat{L}_\alpha \theta + f(\theta)/\tau \qquad (5)$$

where $\hat{L}_\alpha$ is a linear operator accounting for the concentration spreading of test particles evolving according to Lévy flights with exponent α. An α-Lévy flight is an independent increment stochastic process, and the distribution of each increment is a Lévy-stable distribution which exhibits a power law tail $P_\alpha(w) \sim |w|^{-(1+\alpha)}$, with $1 < \alpha < 2$. The moments behave as $\langle |x(t)|^q \rangle \sim t^{q/\alpha}$ for $q < \alpha$ and $\langle |x(t)|^q \rangle = \infty$ for $q > \alpha$. So, the role of ν in Eq. (4) is played by $1/\alpha$ (for $q < \alpha$). Since $1/\alpha > 1/2$, one can speak of anomalous diffusion. Summarizing, we replace the operator $-(\mathbf{u} \cdot \nabla) + D_0 \nabla^2$ in the Eq. (1) by $\hat{L}_\alpha$ substituting an α-Lévy flight to the Eq. (3). Only for simplicity in the notation and in the numerical computation [5,14] we consider a reacting term which is non zero only at discrete time step, when δ-form impulses occur:

$$f(\theta, t) = \sum_{n=-\infty}^{\infty} g(\theta) \delta(t - n\Delta t)\, \Delta t \;, \qquad (6)$$

and we introduce the reaction map $G(\theta) = \theta + \frac{\Delta t}{\tau} g(\theta)$ governing the evolution of an homogeneous field θ (i.e., without diffusion): $\theta(t + 0^+) = G(\theta(t))$. The detailed shape of $G(\theta)$ is not important [5,14], it is just necessary to have an unstable fixed point in $\theta = 0$ and a stable one in $\theta = 1$. In the following we will present the results for the map:

$$G(\theta) = \theta / [\theta + (1 - \theta) \exp(-\Delta t/\tau)] \;. \qquad (7)$$

i.e., the exact solution of the equation $d\theta/dt = \theta(1-\theta)/\tau$. Noting that, assuming Eq. (6), between $t + 0^+$ and $t + \Delta t$ Eq. (5) reduces to the linear equation $\partial_t \theta = \hat{L}_\alpha \theta$, and we can determine the field $\theta(x, t + \Delta t)$ in terms of $\theta(x, t)$:

$$\begin{aligned} \theta(x, t + \Delta t) &= \int_{-\infty}^{+\infty} \mathrm{d}w P_{\alpha,\Delta t}(w) \theta(x - w, t + 0^+) \\ &= \int_{-\infty}^{+\infty} \mathrm{d}w P_{\alpha,\Delta t}(w) G(\theta(x - w, t)) \qquad (8) \end{aligned}$$

where $P_{\alpha,\Delta t}(w)$ is the probability distribution to have a flight of size w in a time interval Δt. Of course $t = n\Delta t$, where n is an integer number. Let us note that, if one assumes the expression (6) for $f(\theta)$, (8) is an exact relation and not only an approximation for small Δt. It is important to stress that using (8) one can avoid the problem of the precise definition of $\hat{L}_\alpha$ in terms of fractional derivative [15,16]. In addition one can study the evolution Eq. (8) using a generic distribution $P_{\alpha,\Delta t}(w)$ which is in the basin of attraction of the α-Lévy stable distribution.

A similar problem has been studied for reaction systems driven by a Lévy walk [17]. In [18] reaction-transport processes using non gaussian random walk for the diffusion process are studied. This approach is similar to our one, but the analysis of [18] is always for a class of processes which give rise to standard diffusion. In addition, in the context of disturbance propagation in chaotic extended systems with long-range coupling, Torcini and Lepri [19] studied a discrete space version of (8) with a linear shape for $G(\theta)$.

Regarding the numerical simulations we study a 1D grid with open boundary conditions and symmetric initial condition with $\theta(x, 0) \neq 0$ in a small region around $x = 0$. We show the results obtained with the reaction map given by Eq.(7) and $\tau = 1$. The principal measured observables are the quantity of inert material, $m(t)$, and the front speed, v_f, defined as:

$$m(t) = \int_{-\infty}^{+\infty} \mathrm{d}x\, \theta(x, t) \qquad v_f = \lim_{t \to \infty} \frac{m(t)}{2t} \;. \qquad (9)$$

Simple arguments suggest that if $P(w)$ is steep enough, e.g., $P(w) \sim \exp(-\beta|w|)$ then the asymptotic behaviour of $\theta(x, t)$ is the usual one of the standard FKPP equation, i.e., $\theta(x, t) \sim h(x - v_f t)$ where $v_f \propto \sqrt{\langle w^2 \rangle}$ and $h(z) \sim \exp(-\gamma z)$ for $z \gg 1$.

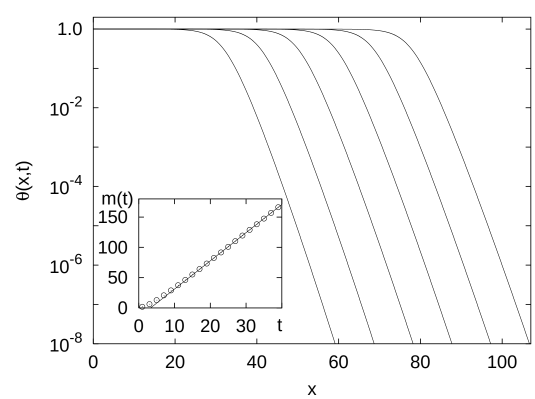

FIG. 1. Front shapes at increasing times in the case of $P(w) \sim \exp(-\beta|w|)$, with $\beta = 1$. The inset shows the quantity of inert material with its asymptotic linear behaviour (solid line). We show just one side of the front.

In this case the inert material increases linearly in time: $m(t) = \mathrm{const} + 2v_f t$ (as for the FKPP equation, see Fig. 1).

More interesting is the case of super-diffusive behaviour with α-Lévy flight ($1 < \alpha < 2$). The shape of $P(w)$ used in the numerical computation is $P(w) = P_0$ for $|w| < w_0$ and $P(w) = P_n |w|^{-(1+\alpha)}$ for $|w| \geq w_0$. The values of the parameters, P_n and P_0, are chosen to guarantee continuity in w_0 and normalization of $P(w)$. Fig. 2 shows that at large time θ develops a power law behaviour $\theta \sim |x|^{-(\alpha+1)}$. In addition, the inert material invades the

fresh one ($\theta \simeq 0$) exponentially fast. This can be seen by looking at the total quantity of inert material at time t,

$$m(t) \sim e^{ct} \tag{10}$$

(see the inset of Fig. 2).

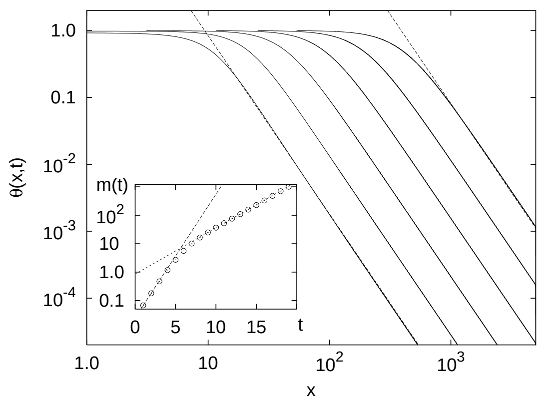

FIG. 2. Front shapes at increasing time in the case of $P(w) \sim |w|^{-(1+\alpha)}$ with $\alpha = \frac{5}{3}$. The dashed lines indicate the theoretical prediction $x^{-(1+\alpha)}$. The inset shows the exponential growth of the inert material. The dotted line is the asymptotic behaviour proportional to $a^{t/(1+\alpha)}$ (see the main text) and the dashed one is the initial rate which grows exponentially as a^t.

The numerical results illustrated above are supported by an analytical argument using a linear analysis of the tail of $\theta(x,t)$ (which is expected to be valid for pulled dynamics [14,20]) and the theory of the infinitely divisible distributions [21]. For θ around zero, $G(\theta)$ has a linear shape $G(\theta) \simeq a\theta$ with $a > 1$. Plugging this into (8), for $x \gg 1$, one has

$$\begin{aligned} \theta(x,t) &\simeq a(P * \theta)(x, t-1) \\ &\simeq a^t (P * P * \cdots * P * \theta)(x, 0) \end{aligned} \tag{11}$$

where $*$ indicates the convolution operation. It is well known [21] that processes with power law tail $P(w) \sim |w|^{-(1+\alpha)}$ with $1 < \alpha < 2$ are in the basin of attraction of the α-Lévy-stable distribution $P_\alpha(w)$. Therefore (11) yields for $|x| \gg 1$ and large t

$$\theta(x,t) \sim |x|^{-(1+\alpha)} a^t \ , \tag{12}$$

in agreement with the behaviour of Figure 2. The growth coefficient in Eq. (10), c, can be computed with a matching argument. We expect (and this is confirmed by simulations) there exists an $\tilde{x}$ value such that $\theta \sim 1$ for $x < \tilde{x}$ and $\theta \sim |x|^{-(1+\alpha)}$ for $x > \tilde{x}$. We can write $m(t) \simeq 2\tilde{x}$, and the value of $\tilde{x}$ can be obtained simply matching the $\theta(x,t)$ in (12) with $\theta \simeq 1$, i.e., $\tilde{x} \sim a^{t/(1+\alpha)} = \exp(\frac{\ln a}{1+\alpha} t)$ and therefore $c = \ln a/(1+\alpha)$, in good agreement with numerical results (see the inset of Fig. 2). The transient, when $\max \theta(x,0)$ is small enough, is dominated by the reaction term, giving an exponential growth $m(t) \sim a^t$.

Particularly interesting is the behaviour for $P(w) \sim |w|^{-(1+\alpha)}$ with $\alpha > 2$. In this case the distribution belongs to the basin of attraction of the gaussian law since $\langle w^2 \rangle < +\infty$ (see [21]). In fact, although the probability distribution, $P(x_t)$, of the sum of independent random variables, $x_t = \sum_{j=1}^t w_j$, has a power law tail, the core of the distribution behaves as a gaussian, and the tail is less and less important as t grows (see Fig. 3). Therefore, at first glance, one could expect the same features of the standard FKPP equation.

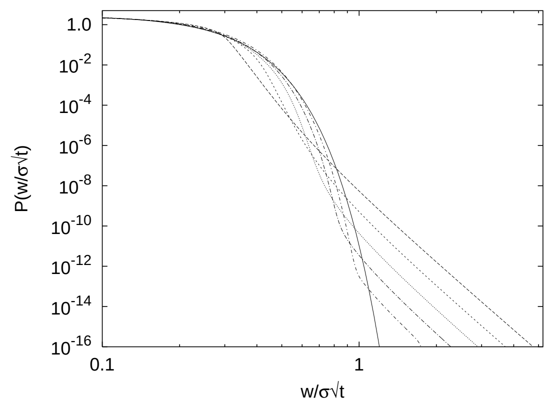

FIG. 3. Rescaled probability density functions, $P(x_t/\sigma\sqrt{t})$, of the sum of independent random variables, $x_t = \sum_{j=1}^t w_j$, in the case of $P(w) \sim |w|^{-(1+\alpha)}$ with $\alpha = 10$ and $t = 2, 4, 8, 16, 32$ from top to bottom; σ is the standard deviation of $P(w)$. The solid line is the gaussian asymptotic behaviour.

But, in reacting systems the presence of this tail can have an important role. In fact for each initial condition, $\theta(x,0)$, localized in a small region (e.g., around $x = 0$), already at the first step, the front has a shape not steep enough for the usual FKPP propagation (i.e., $\theta(x,1) \sim |x|^{-(1+\alpha)}$) [20]. Then, because of the reaction, i.e., the instability of $\theta = 0$, the tail of θ increases exponentially in time. As consequence of the gaussian core of $P(x_t)$ we expect that the bulk of θ behaves in the FKPP way, but, at large time, the exponential growth of the tail has the dominant role.

In Fig. 4 it is shown how, the exponential form of the front (which moves with a constant velocity) is overcome by a power law tail that grows more and more as the time increases, i.e., the initial FKPP behaviour (constant v_f and $\theta(x,t)$ with exponential decay) is replaced by the exponential increasing of the inert material and $\theta(x,t)$ with power law tail. This result is similar to that obtained in [22] in the context of the growth of perturbation in CML: even a weak long range coupling (e.g, a power law with large α) has, at large time, a dramatic effect.

Summarizing, we have shown how, in a reaction diffusion system, replacing a standard diffusion with a process whose probability distribution has a tail approaching to zero faster than a power law, one has the same qualitative

behaviour of the usual FKPP system, i.e., exponential decay of the front and a finite front speed.

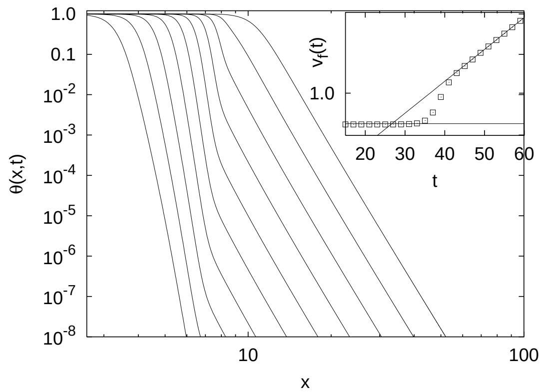

FIG. 4. Front shapes at $t = 19, 22, 25 \cdots$ where $P(w)$ is the same as Figure 3. In the inset it is shown the front speed $v_f(t) = (m(t+1) - m(t))/2$. The straight lines indicate the linear propagation regime, $v_f = cost$, and the exponential propagator regime, $v_f \propto \exp(t \; \ln a/(1+\alpha))$.

On the contrary, if the process has the same tail in the probability distribution of an α-Lévy stable process one achieves an exponentially fast propagation of the front, instead of the linear one. Moreover the tails of the field θ have a power law behaviour instead of the exponential decay. As intermediate behaviour we have the case of a stochastic process whose increment have a power law tail but with finite variance. In this case, initially one has the usual FKPP behaviour, but after a while, one has an exponential growing of the inert material.
Let us now compare the above described scenario with the case of super-diffusion induced by strong time correlation of the velocity field. An example is provided by the standard map with suitable values of the control parameter K [12]. This advection-diffusion system can show super-diffusive behaviour [12] in the limit of $D_0 \to 0$. However in the presence of reaction the front speed is finite for each value of D_0, because it is bounded by $U_{max} + v_0$, where U_{max} is the maximum velocity of the test particle, and v_0 is the front speed in absence of stirring. Therefore, just the presence of anomalous diffusion does not necessarily imply a non-linear front propagation, but also the details of the transport-diffusion and reaction mechanisms are important. For example, in the system (8) using a reaction map with $G(\theta) = \theta$ around $\theta = 0$ (e.g., ignition) we have always the usual scenario shown in Fig. 1 also for $1 < \alpha < 2$.
Such a fact is, in our opinion, relevant for the modeling of realistic reaction systems: one has to mimic precisely the mechanism that gives rise to the anomalous diffusion, beyond the simple power law behaviour of $\langle x^2(t) \rangle$.

We thank M. Cencini, P. Muratore-Gianneschi and A. Torcini for useful discussions and comments. A.V. thanks A.Kupiainen for his kind hospitality at the University of Helsinki during the final write up of this article. This work has been partially supported by INFM *Parallel Computing Initiative* and MURST (*Cofinanziamento Fisica Statistica di Sistemi Complessi Classici e Quantistici*). We acknowledge support from the INFM *Center for Statistical Mechanics and Complexity* (SMC).

[1] J.D. Murray, *Mathematical Biology*, Springer-Verlag, Second Edition, (1993).
[2] J. Xin, SIAM Review **42**, 161 (2000).
[3] N. Peters, *Turbulent combustion*, Cambridge University Press (2000).
[4] A. N. Kolmogorov, I. G. Petrovskii, and N. S. Piskunov, Moscow Univ. Bull. Math. **1**, 1 (1937);
R. A. Fischer, Ann. Eugenics **7**, 355 (1937).
[5] M. Abel, A. Celani, D. Vergni and A. Vulpiani, Phys. Rev. E **64**, 046307 (2001).
[6] P. Constantin, A. Kiselev, A. Oberman and L. Ryzhik, Arch. Rational Mechanics **154**, 53 (2000).
[7] A. J. Majda, and P. R. Kramer, Phys. Rep. **314**, 237 (1999).
[8] P. Castiglione, A. Mazzino, P. Muratore-Ginanneschi, A. Vulpiani, Physica D, **134**, 75 (1999).
[9] G. M. Zaslavsky, D. Stevens and A. Weitzener, Phys. Rev. E **48**, 1683 (1993)
[10] E. Montroll and M. Schlesinger, in *Studies in Statistichal Mechanics* vol.11, Ed.s E. Montroll and J. Lebowitz, page 1 (North-Holland, Amsterdam 1984)
[11] J. Klafter, M. F. Shlensinger and G. Zumofen, Physics Today **49**, 33 (1996)
[12] R. Ishizaki, T. Horita, T. Kobayashi and H. Mori, Prog. Theor. Phys. **85**, 1013 (1991)
[13] G. Falkovich, K. Gawedsky and M. Vergassola, Rev. Mod. Phys. **73**, 913 (2001)
[14] A. Torcini, A. Vulpiani and A. Rocco, Eur. Phys. J. B **25**, 333 (2002)
[15] A.I. Saichev and G. Zaslavsky, Chaos **7**, 753 (1997)
[16] H.C. Fogedby, Phys. Rev. Lett. **73**, 2517 (1994)
[17] G. Zumofen and J. Klafter, Phys. Rev. E **50**, 5119 (1994)
[18] S. Fedotov, Phys. Rev. Lett. **86**, 962 (2001).
[19] A. Torcini and S. Lepri, Phys. Rev. **E 55**, R3805 (1997).
[20] U. Ebert and W. van Saarloos, Physica D **146**, 1 (2000)
[21] B. Gnedenko and A.N. Kolmogorov *Limit distribution for Sums of Indipendent Random Variables*, Addison-Wesley (1954)
[22] G. Paladin and A. Vulpiani J. Phys. A **27**, 4911 (1994)